

Interactive Processes in Sprays - NEL

During the week of the Study Group essentially all attention was focussed on the reactive and diffusive aspects of a burning spray; at this stage the velocity of the droplets and vapour mixture were taken as given. As a further simplification effects of expansion of the vapour, due to vaporisation, thermal effects, and combustion, have, to date, been ignored when considering a bulk or averaged model.

The fuel droplets were taken to act as a source of fuel vapour. Their evaporation rates should be determined by a microscopic analysis of temperature and concentration variations around a single droplet, giving a bulk source of fuel vapour which reacts with oxygen in the air. The distribution of the droplets, i.e. the number of a given size per unit volume, was taken to be specified by the behaviour of the nozzle (including neighbouring turbulence). It was supposed that random variations can result in some regions of air having more or larger droplets, and so being "fuel rich", or fewer or small droplets, and so being "oxygen rich". (The spray is designed so that there is just enough fuel to be burnt by the air.)

Given the earlier simplifications concerning the fluid mechanics and velocities of the system it was decided that, for the present purposes of examining possible chemical behaviour, the fluid/droplet velocity should be taken as zero so a possible averaged model might be:

$$\begin{aligned}\rho C \bar{T}_t &= k \nabla^2 \bar{T} + H \bar{R} - L \bar{E} \\ \bar{c}_t &= D \nabla^2 \bar{c} - \bar{R} + \bar{E} \\ \bar{c}_{0t} &= D \nabla^2 \bar{c}_0 - S \bar{R}\end{aligned}$$

where \bar{T} = averaged temperature (since the mass of fuel $\approx \frac{1}{15}$ mass of air the average can be, approximately, taken over only the gas)

\bar{c} = average mass of vapour/unit volume,

\bar{c}_0 = average mass of oxygen/unit volume.

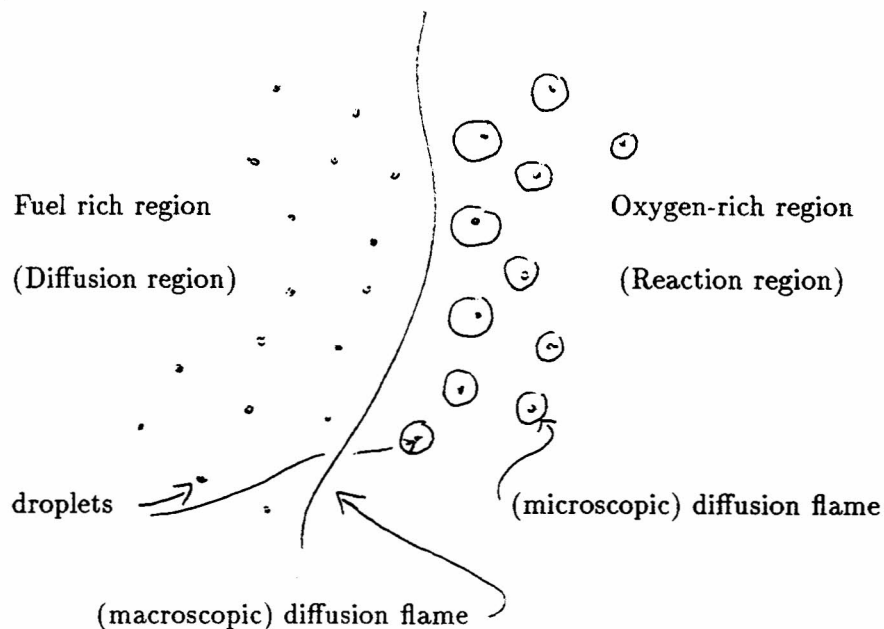
Here: ρ = density of the gas (since we do not allow any expansion due to reaction or increase in temperature and we wish to keep the model as simple as possible we take density of fuel vapour \simeq density of any other vapour present, e.g. nitrogen, \simeq constant); C = specific heat (at constant pressure); k = thermal conductivity of the gas; D = mass diffusivity (again we suppose oxygen and fuel have the same c , k and D); H = heat of reaction (amount

of heat released where one unit mass of fuel is burnt); L = latent heat of vaporisation of the fuel; S = stoichiometric constant (mass of oxygen used in burning a unit mass of fuel). Also \bar{R} = reaction rate (mass of fuel burnt/unit volume/unit time) and \bar{E} = average vaporisation rate (mass of fuel evaporated or boiled from the spray droplets/unit volume/unit time).

For such a model to be meaningful the macroscopic length scale(s), e.g. size of flames, should be much greater than a typical droplet separation (for $\approx 2 \times 10^7$ droplets/m³ this (microscopic) length scale ≈ 4 mm).

There are various parts of the spray of likely interest. In particular near the nozzle the mixture might be cold, so at first evaporation of the fuel can occur without appreciable reaction. The gaseous mixture of fuel and oxygen can then burn as a premixed flame. We restrict our attention to some time (or rather place) beyond this, where the mixture is hot. Taking the reaction to be first order in both fuel and oxygen (local) reaction rate = $cc_0F(T)$ where now $F(T)$ is large (typically F will be Arrhenius, $F(T) = KT^n \exp(-E/RT)$, E = activation energy - typically "large" - and R = universal gas constant). This means we can expect $c \approx 0$ (oxygen rich, fuel depleted) or $c_0 \approx 0$ (fuel rich, oxygen depleted) in separate regions with a flame between the two. This is classical diffusion flame behaviour. The picture envisaged is sketched in figure 1.

Figure 1. Large scale diffusion flame between fuel-rich and oxygen-rich regions.



In the left hand region — the diffusion region — fuel vaporises and diffuses but there is no combustion:

$$\begin{aligned}\rho C \bar{T}_t &= k \nabla^2 \bar{T} - L \bar{E} \\ \bar{c}_t &= D \nabla^2 \bar{c} + \bar{E} \text{ (and } \bar{c}_0 \approx 0) .\end{aligned}$$

In the right hand region — the reaction region — fuel vaporises and is quickly burnt near each droplet. Each droplet is surrounded by its own small diffusion flame. These flames burn at the same rate as the vaporisation so $\bar{R} = \bar{E}$ (and they also cause oxygen depletion at the corresponding rate. Outside of these $\bar{c} \approx 0$ and oxygen diffuses:

$$\begin{aligned}\rho C \bar{T}_t &= k \nabla^2 \bar{T} + (H - L) \bar{E} \\ \bar{c}_{0t} &= D \nabla^2 \bar{c}_0 - S \bar{E} \text{ (and } \bar{c} \approx 0).\end{aligned}$$

To complete the model it is necessary to know the change of droplet size and so determine \bar{E} .

We take $n(x, t, m)$ to be the volumetric number density of particles of mass m around position x at time t (the number of particles with masses between m_1 and m_2 in a region of volume V and which is small compared to the macroscopic scale but large on the microscopic scaling around x is $V \int_{m_1}^{m_2} n(x, t, m) dm$). Then the rate of change of n is given by

$$n_t = \frac{\partial}{\partial m}(nf) \quad m > 0$$

where f is the rate of loss of mass (vaporisation rate) of a particle of size m . An individual particle has mass changing according to $\dot{m} = m_t = -f$. The vaporisation rate could depend on T (temperature of the gas near the drop) and concentrations c or c_0 . (Increased T should result in higher heat flow into the drop and consequent higher boiling rate; increased c_0 should give higher oxygen flow into the flame and faster burning and vaporisation of the fuel.) The total vaporisation rate \bar{E} , from conservation of mass of fuel, must be

$$\bar{E} = -\frac{dM}{dt}$$

where $M = \int_0^\infty m n dm =$ mass of droplets per unit volume. Differentiating under the integral sign, $-\frac{dM}{dt} = -\int_0^\infty m n_t dm = -\int_0^\infty m \frac{\partial}{\partial m}(nf) dm$ (from the above) $= \int_0^\infty n f dm - [m n f]_0^\infty$ on integrating by parts. Assuming that $m n f = 0$ both for $m = 0$ (which, if n is bounded, is the case for the evaporation law derived below) and $m = \infty$ (which will be true if n decays rapidly enough as $m \rightarrow \infty$) then we also have

$$\bar{E} = \int_0^\infty n f dm.$$

(A discrete version of this is given by coagulation – fragmentation equations, for which a term corresponding to mnf at $m = 0$ can be significant.)

Since this analysis is supposed to refer to a region where significant heating has already occurred we take the droplets to have boiling temperature T_B . The rate of vaporisation f is determined by the rate of arrival of heat.

Trying to proceed upon the assumption that boiling is controlled purely by diffusive mechanisms appears to lead to some unrealistic predictions so we are forced, at least in the neighbourhood of individual drops, to allow for mass flow away:

$$\begin{aligned} u &= \text{velocity of vapour away from the droplet} \\ &= f/4\pi\rho r^2 \end{aligned}$$

where r = distance from the drop's centre (we assume local radial symmetry).

Also mass flow away = $f = 4\pi r^2(uc - Dc_r)$, where c is the local mass of fuel vapour per unit volume.

At this stage we make, for convenience, another simplifying assumption, namely that the Lewis number is one (i.e. the diffusivity of fuel and oxygen is the same as that of heat):

$$D = k/\rho C$$

Then both concentration and temperature satisfy the same equation:

$$\left. \begin{aligned} \frac{\partial}{\partial r}(r^2(uc - Dc_r)) &= 0, \\ \frac{\partial}{\partial r}(r^2(uT - DT_r)) &= 0, \\ \text{and } c_0 &= 0, \end{aligned} \right\} a < r < b$$

where we assume for the moment that there is a (diffusion) flame at $r = b$. The boundary $r = a$ represents the droplet surface and so

$$T = T_B \text{ and } Lf = 4\pi a^2 k T_r \text{ at } r = a.$$

The latter condition equates inflow of heat with that used in boiling the liquid (there is no temperature gradient within the droplet).

Outside the flame

$$\text{and } \left. \begin{aligned} c &= 0; \\ \frac{\partial}{\partial r}(r^2(uT - DT_r)) &= 0; \\ \frac{\partial}{\partial r}(r^2(uc_0 - Dc_{0r})) &= 0; \end{aligned} \right\} r > b .$$

All four different equations have solutions of the form

$$y = A + B \exp(-f/4\pi\rho D r)$$

giving, in total, eight constants of integration, one of which can be taken to be f . Additionally, the flame radius b is an unknown.

As well as the two conditions on $r = a$ we have the conditions at infinity: away from the droplet temperature \simeq average temperature, oxygen concentration \simeq average oxygen concentration, i.e.

$$c_0 \rightarrow \bar{c}_0 \text{ and } T \rightarrow \bar{T} \text{ as } r \rightarrow \infty.$$

The usual diffusion flame conditions hold at $r = b$:

$$\begin{aligned} [T] &= 0 && \text{(temperature is continuous)} && ; \\ c = c_0 &= 0 && \text{(concentrations approach zero)} && ; \\ Sc_r + c_{0r} &= 0 && \text{(stoichiometry)} && ; \\ k[T_r] &= HDc_r && \text{(heat of reaction)} && . \end{aligned}$$

These five conditions at $r = b$, together with the two each at $r = a$ and $r = \infty$, are sufficient to determine b and the eight constants of integration. In particular

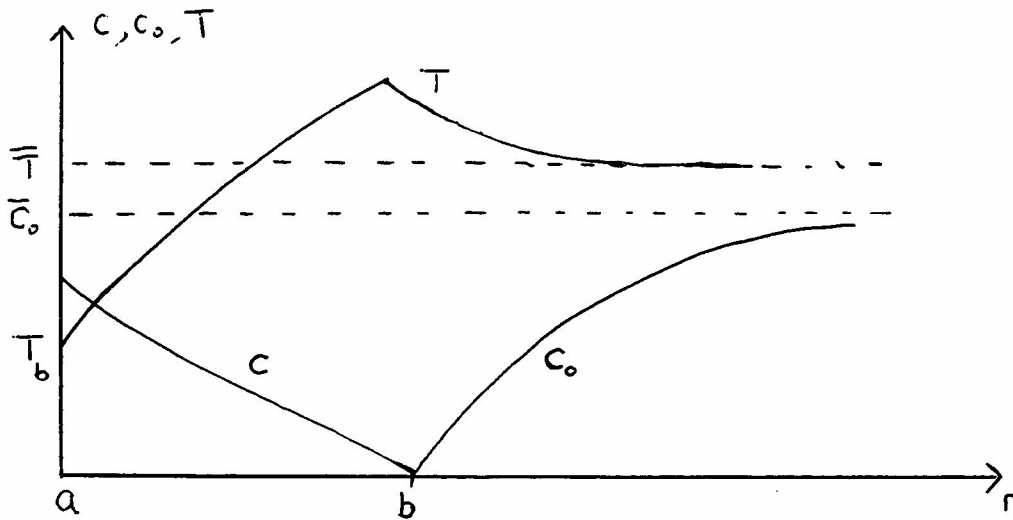
$$f = 4\pi\rho Da \ln \left[1 + \frac{C}{L}(\bar{T} - T_B + H\bar{c}_0/S\rho C) \right] ,$$

or, using $m = \frac{4}{3}\pi\rho_l a^3$, where ρ_l = density of liquid fuel,

$$f = 4\pi\rho D \left(\frac{3m}{4\pi\rho_l} \right)^{1/3} \ln \left[1 + C(\bar{T} - T_b + H\bar{c}_0/S\rho C)/L \right].$$

The temperature and concentrations are sketched in figure 2.

Figure 2. Temperature and concentrations near a droplet.



The vaporisation rate in the diffusion region is given simply by setting $\bar{c}_0 = 0$ in the above expression (f can be calculated independently of \bar{c} , which, along with c , should be no greater than ρ). The above equation (with or without \bar{c}_0) was given in the review article [1] although there it did not appear clear as to the constants were.

We now take the ideal case of the droplets in a small region all having the same size, $m(x, t)$, with number density $N = N(x) = 0(N_0)$, $N_0 \simeq 2 \times 10^{+7} m^{-3}$.

Then in the diffusion region ($\bar{c}_0 = 0$)

$$\begin{aligned}\bar{T}_t &= D \nabla^2 \bar{T} - L\bar{E}/\rho C \\ \bar{c}_t &= D \nabla^2 \bar{c} + \bar{E} \\ \bar{E} &= Nf = -N\dot{m} \quad , \\ \dot{m} = -f &= -4\pi\rho D \left(\frac{3m}{4\pi\rho_l}\right)^{1/3} \ln\left[1 + \frac{C}{L}(\bar{T} - T_B)\right] \quad , \\ &\text{or,}\end{aligned}$$

$$\begin{aligned}\bar{T}_t &= D \nabla^2 \bar{T} + \frac{LN}{\rho C} m_t \quad , \\ \bar{c}_t &= D \nabla^2 \bar{c} - N m_t \quad , \\ \dot{m} = m_t &= -4\pi\rho D \left(\frac{3m}{4\pi\rho_l}\right)^{1/3} \ln\left[1 + \frac{C}{L}(\bar{T} - T_B)\right] \quad ,\end{aligned}$$

while in the reaction region ($\bar{c} = 0$)

$$\begin{aligned}\bar{T}_t &= D \nabla^2 \bar{T} - \frac{(H-L)N}{\rho C} m_t \quad , \\ \bar{c}_{0t} &= D \nabla^2 \bar{c}_0 + SN m_t \quad ; \\ \dot{m} = m_t &= -4\pi\rho D \left(\frac{3m}{4\pi\rho_l}\right)^{1/3} \ln\left[1 + \frac{C}{L}(\bar{T} - T_B + \frac{H\bar{c}_0}{S\rho C})\right]\end{aligned}$$

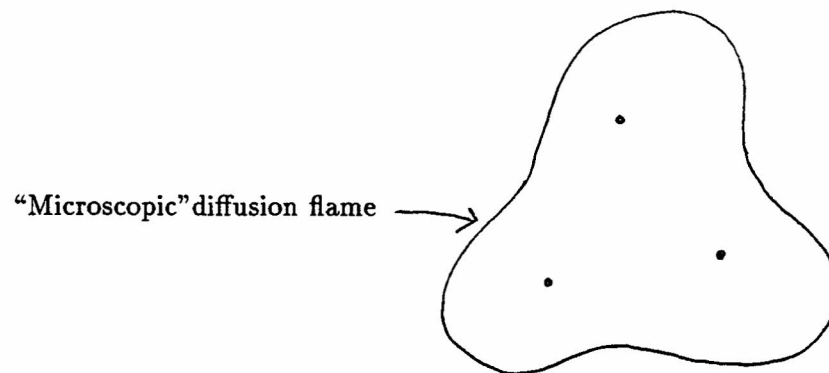
Between these two regions there is a macroscopic diffusion flame where

$$\begin{aligned}\bar{c} &= \bar{c}_0 = 0 \quad , \\ [\bar{T}]_a^r &= 0 \quad , \\ S \frac{\partial \bar{c}}{\partial \nu} + \frac{\partial \bar{c}_0}{\partial \nu} &= 0 \quad , \\ k \left[\frac{\partial \bar{T}}{\partial \nu} \right]_d &= HD \frac{\partial c}{\partial \nu} \quad ;\end{aligned}$$

here $\frac{\partial}{\partial \nu}$ denotes the normal derivative into the reactive region.

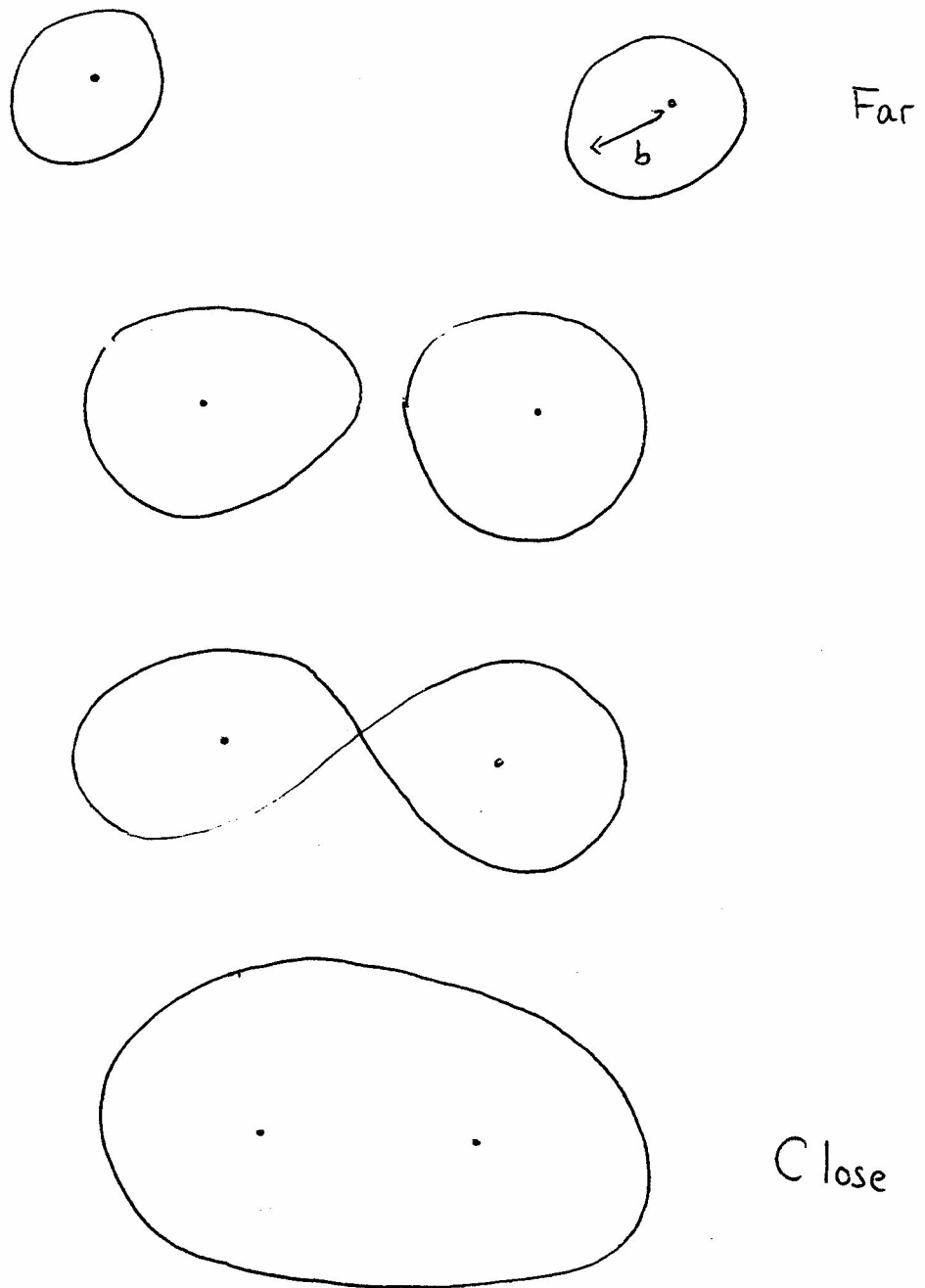
There was some speculation that there could be some type of “mushy region” with clusters of a few (or several) droplets surrounded by a small flame (see figure 3).

Figure 3.A three-droplet cluster.



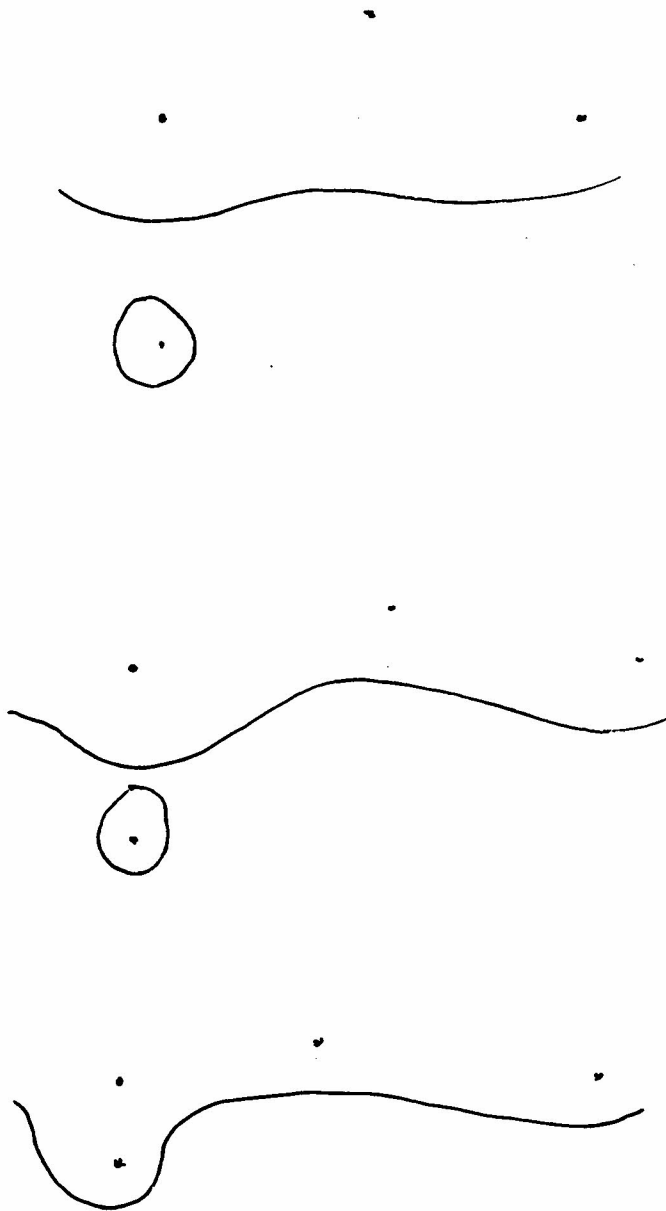
Such a phenomenon was suggested in [1]. It was also motivated by noting that near a droplet oxygen is depleted so as two approached the flames are likely to extend towards each other and eventually merge (see figure 4).

Figure 4. Two approaching or separating drops.



In the same way a drop and its flame could coalesce (or separate from) a larger cluster or the macroscopic diffusive region (see figure 5).

Figure 5. A droplet and flame near the macroscopic diffusive flame.



This scenario was not considered further.

The equations can be normalized. It appears appropriate to nondimensionalize \bar{c} with initial mass of (liquid) fuel per unit volume: $\bar{c} = M_0 c = N_0 m_0 c$ ($N_0 =$ original number density, $m_0 =$ original average droplet mass); temperature with the rise due to complete burning: $\bar{T} = T_B + \frac{HM_0}{\rho C} T$ (note that we are only considering later stages of the process when temperature is above the boiling point of the fuel; we should emphasize that for earlier times — lower temperatures — a different vaporisation law might apply); oxygen concentration with that needed to burn all the fuel: $\bar{c}_0 = SM_0 c_0$ (of course this means scaling with oxygen concentration in air since M_0 is chosen to get complete reaction of both fuel and oxygen).

The logarithmic term appearing in the vaporisation rates then becomes

$$\ln[1 + \beta(T + C_0)]$$

where $\beta = \frac{HM_0}{L\rho} \simeq 100$ (this essentially indicates the large value of heat of reaction compared to latent heat). With such a large β we may take, for most of the region of interest,

$$\ln[1 + \beta(T + c_0)] \simeq \ln \beta \simeq 5 \quad .$$

This approximation fails where $T + c_0$ is small, which is likely only to happen in the diffusive region. For $c_0 = 0$ and $T \ll 1/\beta$ $\ln[1 + \beta T] \simeq \beta T$.

There was some discussion of travelling wave solutions. We look at a one-dimensional (after averaging) problem with the flame moving towards the diffusive region (say in the negative x - direction); this seems most appropriate physically as we would like the drops to move towards the flame, away from the nozzle.

A dimensionless problem is then

Diffusion region , $z < 0$:

$$VT' = T'' + V\gamma M' \quad ; \quad Vc' = c'' - VM' \quad ; \quad -VM' = \alpha M^{1/3} \ln(1 + \beta T) \quad .$$

Diffusion flame , $z = 0$:

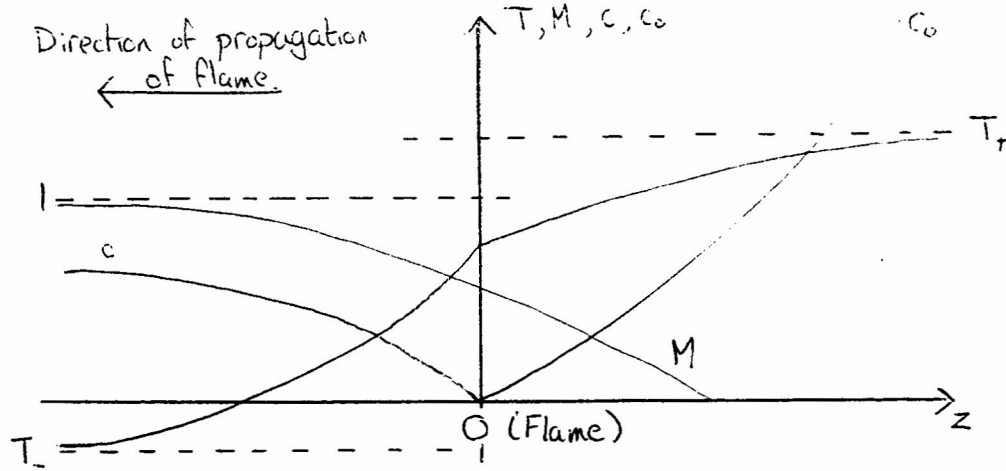
$$c = c_0 = 0 \quad ; \quad [T] = 0 \quad ; \quad c' + c'_0 = 0 \quad ; \quad [T']_{\pm} = c' \quad .$$

Reaction region , $z > 0$:

$$VT' = T'' + V(\gamma - 1)M' \quad ; \quad Vc'_0 = c''_0 + VM' \quad ; \\ -VM' = \alpha M^{1/3} \ln(1 + \beta(T + c_0)) \quad .$$

Possible profiles are sketched in figure 6.

Figure 6. Temperature and concentrations for a travelling wave.



Here z is the scaled travelling wave variable (distance behind the flame), V is the dimensionless speed of the flame relative to the vapour, and $\gamma = L/H \ll 1$. Using $\gamma \ll 1 \ll \beta$ some simplification of this system is likely to be possible. It certainly appeared that even for a more general problem there were solutions satisfying $M \rightarrow 1$ and $T \rightarrow T_- \leq 0$ for $z \rightarrow -\infty$. It was not checked that we would have $T \rightarrow T_+ = T_- + 1 > 0$ as $z \rightarrow \infty$. (It was observed that, as with a conventional diffusion flame, $c_0 \rightarrow \infty$ as $z \rightarrow \infty$.) It is clear that M reaches 0 at a finite value of z (possibly negative so drops completely vaporise before they can reach the flame). It might also be possible, using the sizes of β and γ , to consider a distribution of droplet sizes in a fairly straightforward manner.

Other aspects of the problem which might be relatively amenable to similar modelling are:

1. The possible mushy region. The time scale involved, is $0(d^2/D)$ where $d =$ typical droplet separation $\simeq 4 \times 10^{-3} \text{m}$, $D =$ diffusivity $\simeq 10^{-4} \text{m}^2 \text{s}^{-1}$ [1], i.e. $0(10^{-1} \text{s})$. This can be compared with time scale for droplet vaporisation, $0(a^2 \rho_l / \rho D)$, taking now a to be a typical drop radius. Given that system is set up so that $a^3 \rho_l \simeq \frac{1}{15} d^3 \rho$ (mass of gas/unit volume is comparable to mass of fuel/unit volume), this latter time scale is $0(d^3 / 15aD) = 0(\frac{d}{15a} \times 10^{-1} \text{s}) = 0(3 \times 10^{-1} \text{s})$, on taking $a \simeq 10^{-4} \text{m}$. The closeness of the timescales suggests that the earlier calculations of vaporisation rate, which come from a quasisteady theory, might need to be examined more carefully.
2. The effect of expansion and separation of the droplets through the effects of boiling, thermal expansion, and combustion.

3. The way in which the gas and drops get warmer, possibly including a premixed flame, and certainly allowing for evaporation rather than boiling.

References

- [1] K Annamalai and W Ryan, "Interactive processes in gasification and combustion. Part I: Liquid drop arrays and clouds." *Prog. Energy Combust. Sci.*, 18 (1992) 221-95.

CA, JC, ADF, NF, MG, JRK, AAL, CPP, JADW